CONFIDENTIAL

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HUMAN HEALTH AND ENVIRONMENTAL ASSESSMENT

of

SILRES® BS 1703

[redacted]

1 IDENTITY

1.1 Identification of the Polymer

[redacted]

lowest number average molecular weight:	1086
maximum weight % below 500 molecular weight:	0.87
maximum weight % below 1000 molecular weight::	31.57
Trade name:	SILRES® BS 1703

1.2 Physico-Chemical properties

[redacted] has a number average molecular weight Mn of 1086 g/mol, and contains a high fraction (~31.57%) of low molecular weight species < 500 g/mol.

Based on data available for the monomer [redacted] (t½ = 0.9 h, pH 4, 20-25 °C; t½ = 43 h, pH 7, 20-25 °C; t½ = 0.5 h, pH 9, 20-25 °C, (Q)SAR) the reaction with water is expected to be moderately fast. However, it should be noted that during product cure, further condensation must be expected, which will lead to an increased average molecular weight, a lower fraction of low molecular weight species, and thus an increased Kow with a decrease in water solubility, and bioavailability.

The vapor pressure of polymers, in general, is low. In this case already the monomer [redacted] has a very low vapor pressure of 0.14 to 0.22 Pa at 20 and 25°C[1]. With subsequent polymer chain increase the vapor pressure rapidly decreases to very low values as can be calculated by MPBPWIN v1.43 (see table 1 and annex I). For the siloxane dimer a vapor pressure of only 0.00009 Pa is predicted. Despite all uncertainties the prediction may have, this indicates that exposure to the polymer by vapor inhalation is negligible.

Table 1: Measured and/or predicted vapor pressure of the monomer [redacted]

Substance (Method)	Result
[redacted] (OECD 104, effusion method)	0.22 Pa @ 25°C
[redacted] (MPBPWIN v1.43)	0.99 Pa @ 25°C
[redacted] (MPBPWIN v1.43)	0.00009 Pa @ 25°C

[1] https://echa.europa.eu/de/registration-dossier/-/registered-dossier/16000/4/7

2 HUMAN HEALTH HAZARDS

The new polymer has not been tested for acute or chronic toxicity. However, the monomer [redacted] has been intensively evaluated in Europe within REACH[2]. Based on the physical-chemical properties of the polymer it is reasonable to identify the monomer as a worst case structural surrogate for the notified polymer. Thus, in the following sections the toxicological data for the monomer are presented and discussed.

2.1 Effects on Human Health

2.1.1 Toxicokinetics, Metabolism and Distribution

No data available.

2.1.2 Acute Toxicity

Studies in Animals

Inhalation

No data are available for the inhalation route for the the monomer [redacted]. Therefore, data are read-across from the related substance [redacted]. The monomer and [redacted] are close structural analogues and both hydrolyse (with predicted half-lives at pH 7 of 43 hours and 5 hours, respectively) to give [redacted]. The other hydrolysis products are ethanol and methanol, respectively.
In a good quality study (Hoechst, 1986a) exposure of Wistar rats to an aerosol of [redacted] at a concentration of 11.2 mg/l air did not cause any deaths. Therefore the LC50 was greater than 11.2 mg/l.

Dermal

An acute dermal toxicity study was conducted with the monomer [redacted] according to OECD 402 on rats. The LD50 (rat) was greater than 2000 mg/kg (BSL, 2001a). The study was carried out in compliance with GLP. There were no clinical signs of toxicity and no abnormalities detected at scheduled necropsy.

Oral

An acute oral toxicity study was conducted with the monomer [redacted] according to OECD 423 on rats. The LD50 (rat) was greater than 2000 mg/kg (RCC Ltd., 1998). The study was carried out in compliance with GLP. There were no clinical signs of toxicity and no abnormalities detected at scheduled necropsy

Based on the available acute oral, dermal and inhalation toxicity studies, the monomer [redacted] is not classified for acute toxicity according to GHS.

[2] https://echa.europa.eu/de/registration-dossier/-/registered-dossier/16000/1

Studies in Humans

No data available.

2.1.3 Irritation

Skin Irritation

Studies in Animals

An acute dermal irritation study was conducted with the monomer [redacted] according to OECD 404 on rabbits (BSL Bioservice, 2000a). The study was carried out in compliance with GLP. The findings of the study did not meet the GHS criteria for classification as irritating to skin.

Studies in Humans

No data available.

Eye Irritation

Studies in Animals

An acute eye irritation study was conducted with the monomer [redacted] according to OECD 405 on rabbits (BSL Bioservice (2001b)). The study was carried out in compliance with GLP. The findings of the study did not meet the GHS criteria for classification as irritating to the eyes.

Studies in Humans

No data available.

Respiratory Tract Irritation

No data available.

2.1.4 Sensitisation

Studies in Animals

The monomer [redacted] was not sensitising in a guinea pig maximisation test carried out in accordance with OECD 406 and in compliance with GLP (BSL Bioservice, 2001c). No positive skin reactions were observed.

2.1.5 Repeated Dose Toxicity

Studies in Animals

Inhalation

No repeated dose inhalation toxicity data are available for the monomer [redacted]. Thus, good quality data for the read-across substance [redacted], have been used to assess the repeated dose inhalation toxicity of [redacted]. The monomer and [redacted] are close structural analogues and both hydrolyse (with predicted half-lives at pH 7 of 43 h and 5 h, respectively) to give [redacted]

[redacted]. The other hydrolysis products are ethanol and methanol, respectively.

In a 28-day inhalation study with [redacted] which was conducted according to OECD 412 and in compliance with GLP (Hoechst, 1986b), four groups of 10 males and 10 females rats were exposed to [redacted] at concentrations of 0, 0.3, 1.5 and 3 mg/l for 28 days (6 hours/day, 5 days/week). After the exposure period five male and five female rats of each group were kept during a 14 day recovery before necropsy. Only some clinical signs have been observed shortly after exposure in the high and mid dose group. There were no treatment related effects on hematology, clinical chemistry, urinalysis, organ weights and gross pathology. There were signs of minimal alveolar irritation (isolated and small clusters of foam cells) in several high dose animals. Overall the NOAEC for this study was considered to be 3 mg/l. Based on gravimetric and chemical verification of the exposure concentrations it can be concluded that animals were exposed to a mixture of aerosol/vapour and therefore systemic availability of the substance is expected.

Oral

A 90-day oral repeated dose toxicity study was conducted with the monomer [redacted] according to OECD 408 and in compliance with GLP. Four groups of 10 male and 10 female rats were dosed via gavage with 0, 15, 50 and 150 mg/kg bw/day for 90 consecutive days. There were no treatment related findings in any of the animals. Thus, the NOAEL of this study was established to be 150 mg/kg bw/day (the highest dose tested) (BSL BioService, 2015).

This subchronic study is supported by two reliable short term (subacute) repeated dose toxicity studies with the monomer [redacted]. The first (CERI, 2001) was a 28-day oral (gavage) study conducted in male and female rats, with a 14-day recovery period. The study was conducted according to OECD 407 and in compliance with GLP. The study identified an NOEL value of 40 mg/kg bw/day, with bladder and liver effects, possibly reversible, at the LOAEL of 200 mg/kg bw/day. Dosing was performed 7 days per week. The second study (BSL Bioservice, 2001d), was conducted according to OECD 407, and in compliance with GLP. The NOAEL for Wistar rats was determined to be 150 mg/kg bw/day for the oral route. There were treatment and dose-related changes in the keratinised gastric mucosa in male rats, the change being present in all dose groups (male high, medium and low, and female high, medium and low dose groups 5/5, 4/5, 2/5 and 1/5, 3/5, 1/5, respectively). In female rats the changes were detected at a lesser frequency and only a ‘minimal’ severity. The associated changes were acanthosis and hyperkeratosis.

In these two subacute (28-days repeated) oral toxicity studies different strains of rats and different vehicles for substance application were used. Based on these differences, the partially different behaviour of the substance in these two tests can be explained (strain specific effects, normal biological variation, different resorption due to different vehicles). Nevertheless, in general no severe systemic toxicological effects were observed in either test.

Changes in the liver (both tests) can be described as an adaptative response to the substance because of metabolism of the parent substance and/or the hydrolysis products, especially ethanol. Irritation effects of the substance were observed on the keratinized gastric mucosa (BSL Bioservice, 2001d) and on the transitional epithelium of the bladder (CERI, 2001). There is an indication of reversibility of the effects.

Different NOAELs were defined in these two tests, which can be explained by the different dose levels selected for each. Effects in the 200 mg/kg dose group (CERI, 2001) were without

morphological findings (relative liver weight) or were very slight to slight in few animals only (hyperplasia of transitional epithelium of the bladder).

Note: Based on the findings of the key study (subchronic 90-day oral repeated dose toxicity study), bladder epithelial hyperplasia findings in the supporting oral subacute toxicity studies of similar degree of severity and missing recovery data have been re-evaluated as being non-adverse.

Based on the available data, the monomer [redacted] is not classified for specific target organ toxicity according to GHS.

Studies in Humans

No data available.

2.1.6 Mutagenicity

Information is available for the monomer from reliable studies for in vitro mutagenicity to bacteria and cytogenicity, and from an in vivo micronucleus assay. No information is available for the monomer for in vitro mutagenicity to mammalian cells; however, data are available for the structural analogue, [redacted].

In vitro Studies

Studies in Bacteria

The monomer [redacted] has been tested in a valid and reliable study conducted according to OECD TG 471 and in compliance with GLP (RCC Cytotest Cell Research, 1998). No mutagenic effect was observed for the test substance tested up to limit concentration in any of the Salmonella typhimurium strains TA 1535, TA 1537, TA 98, TA 100 and TA 102 in a plate incorporation experiment without and with metabolic activation. The result was confirmed in an independent pre-incubation assay. Appropriate positive, negative and solvent controls were included and gave expected results. It is concluded that the test substance is negative for mutagenicity to bacteria under the conditions of the test.

Studies in Mammalian Cells

The monomer [redacted] has been tested in a valid and reliable test performed according to OECD TG 473 in compliance with GLP (BSL Bioservice, 2001e). The test substance did not induce structural chromosomal aberrations in the V79 Chinese hamster cell line with and without metabolic activation up to limit concentrations. Appropriate solvent and postive controls were included and gave expected results. It is concluded that the test substance is negative for the induction of chromosome aberrations under the conditions of the test.

An additional study on in vitro cytogenicity with the monomer [redacted] is available (CERI Japan, 2001). This study reported a positive in Chinese hamster fibrobalsts (V79 cells) in the absence of metabolic activation. The study report available for this result is an extended summary, and does not include tables of results, so there is not enough information to for a full independent assessment, but it is noted by the reviewer that the test substance was much more cytotoxic in the absence of activation, and the increase in abnormalities recorded was most marked at cytotoxic concentrations. In view of

these factors, the availability of a reliable negative result in a similar study and the negative result in vivo, the study with the negative result was chosen as key.

Information on mutagenicity to mammalian cells is available for a structural analogue of the monomer, [redacted] which has been tested in a reliable study conducted according to OECD TG 476 and in compliance with GLP (Bioservice, 2012). No biologically relevant increase in mutation rate was found in mouse lymphoma L5178Y cells with or without metabolic activation in either the initial or the repeat experiment, up to limit and cytotoxic concentrations. The global evaluation factor was not exceeded at any concentration. In addition, colony sizing showed no clastogenic effects in either experiment. Appropriate solvent and positive controls were included and gave expected results. It is concluded that the test substance is negative for mutagenicity to mammalian cells under the conditions of the test.

In vivo Studies

The monomer [redacted] has been tested in a reliable in vivo mouse micronucleus assay according to OECD 474 and under GLP (Bioservice (2001)). No statistically significant increase in the number of cells with micronuclei was observed after oral administration of the limit dose of 2000 mg/kg bw. Appropriate positive and vehicle controls were included and gave expected results. The PCE / NCE ratio was slightly affected in treated males, indicating that the test item was of low toxicity to the target tissue. It is concluded that the test substance is negative for the induction in micronuclei under the conditions of the test.

2.1.7 Carcinogenicity

No data available.

2.1.8 Toxicity for Reproduction

Effects on Fertility

No data are available for the monomer [redacted] to assess effects on fertility. Thus, good quality data for a structural analogue of the monomer [redacted], have been used to assess effects on fertility of [redacted].

In a guideline, GLP, OECD 422 study (DCC, 2010) for the related substance [redacted], reproductive effects (increased duration of gestation, dystocia, decreased pup viability on PND 0 and 4, mean litter weights, average pup body weights and body weight gain decreased on PND 4) were only observed at the highest dose of 1000 mg/kg bw/day and were considered to be secondary to the systemic toxicity in dams (including dragging of hindlimbs) by the study authors. There were no effects on fertility. The NOAEL is therefore ≥ 1000 mg/kg bw/day.

Developmental Toxicity

The monomer [redacted] has been tested in a reliable developmental toxicity study conducted in accordance with OECD 414 and in compliance with GLP (Harlan (2009a)). Under the conditions described for this study, the NOEL for pregnant rats was considered to be ≥1000 mg/kg body weight/day. Based on the variations on

development of axial skeleton, the NOEL for embryo and fetal development was considered to be 100 mg/kg body weight/day whereas the NOAEL was considered to be ≥1000 mg/kg body weight/day.

This is supported by a reliable OECD 422 study with the related substance [redacted] in which the NOAEL was ≥1000 mg/kg bw/day (Dow Corning Corporation, 2010).

Based on the available data, the monomer [redacted] is not classified for reproductive or developmental toxicity according to GHS.

3 HAZARDS TO THE ENVIRONMENT

The new polymer has not been tested for acute or chronic aquatic toxicity. However, the monomer [redacted] has been intensively evaluated in Europe within REACH . Based on the physical-chemical properties of the polymer it is reasonable to identify the monomer as a worst case structural surrogate for the notified polymer. Thus, in the following sections the ecotoxicological data for the monomer are presented and discussed.

As supporting information chronic ecotoxicity values have been calculated by ECOSAR(V 1.11) for the ecotoxicologically relevant hydrolysis products.

No effects on aquatic organisms are expected from the hydrolysis product ethanol.

3.1 Aquatic Effects

Acute Toxicity Test Results

For the monomer short-term toxicity tests results are available for freshwater fish (Oncorhynchus mykiss), invertebrates (Daphnia magna) and algae (Pseudokirchneriella subcapitata), (IBACON (2001a), IBACON (2001b), IBACON (2001c), IBACON (2001d), Harlan (2010b)). However, in all these studies the loading rates were well above the water solubility of the monomer (<0.1 mg/l). The observations during the tests with fish, Daphnia and algae indicated that the dosage of the test item and the filtration step are hypersensitive parameters for the occurrence of undissolved material. A cellulose-acetate filter, as was used in these studies, is not able to retain effectively undissolved monomers and oligomers. Therefore, reliable data of the structural analogue, [redacted] have been used to assess the acute aquatic toxicity of the monomer. For all 3 trophic levels the studies were performed up to the solubility limit of the structural analogue, [redacted] not achieving any toxicity (Springborn Smithers (2008a), Springborn Smithers (2008b), Springborn Smithers (2008c)).

The relevant short-term values are:

Fish (*Oncorhynchus mykiss*): LC50 (96-h): >0.055 mg/l; NOEC: ≥0.055 mg/l (based on nominal concentrations).

Daphnia (*Daphnia magna*): EC50 (48-h): >0.049 mg/l; NOEC: ≥0.049 mg/l (based on nominal concentrations).

Algae (*Pseudokirchneriella subcapitata*): ErC50 (72-h): >0.13 mg/l; NOEC: ≥0.13 mg/l (based on nominal concentrations).

Thus, the structural analogue, [redacted] did not achieve any toxicity in all 3 trophic levels when tested at the solubility limit.

Chronic Toxicity Test Results

For the monomer a chronic aquatic toxicity test result is available for invertebrates (Daphnia magna), (Harlan (2010a)). However, like in the case of the short-term aquatic toxicity studies mentioned above the loading rate was well above the water solubility of the monomer (<0.1 mg/l). Therefore, it is not possible to separate physical from systemic effects at the effect concentrations and to quantify a reasonable no effect concentration (NOEC) for the monomer and its hydrolysis products from this study.

Therfore, as supporting information chronic ecotoxicity values have been calculated by ECOSAR (V 1.11) for the ecotoxicologically relevant hydrolysis products. The result is shown in table 2 exemplarily for the monomeric [redacted] and the corresponding tetramer (Full report see Annex II).

Table 2: ECOSAR (V1.11) chronic results for the ecotoxicologically relevant hydrolysis products (HP), exemplarily calculated for [redacted] and the corresponding siloxane tetramer (Molecular Weight approx. 715)

ECOSAR Endpoint	Result Monomer HP [mg/L]	Result Tetramer HP [mg/L]
Fish (ChV)	136	1.22e-005 *
Daphnid (ChV)	59	4.56e-005 *
Green Algae (ChV)	82	0.00122 *

* the asterisk designates that for all 3 trophic levels the predicted effect level exceeds the water solubility by >10x and the predicted log Kow for the tetramer is greater than the endpoint specific cut-off of 8.0 for ChV.

Based on the ECOSAR (V1.11) predictions no chronic effects on aquatic organisms are expected for the polymer, the residual monomer and its hydrolysis products.

3.2 Other Environmental Effects

Biodegradation in water

Two reliable guideline studies are available for the monomer (Clarke (2009), Hertl (2001)). The most recently-conducted study was chosen as the key study. 13% biodegradation in 28 days was determined in a reliable study conducted according to an appropriate test protocol (OECD 301), and in compliance with GLP. The supporting study indicated 0% to 2% biodegradation in 28 days (OECD 301 F). This study was also conducted in compliance with GLP.

The monomer [redacted] is expected to hydrolyse within the timescale of the ready biodegradation study (half-life 43 hours at pH 7 and 20-25°C, predicted) to [redacted] and ethanol. Ethanol is readily biodegradable (OECD, 2004). Therefore a biodegradation of ~40% would be expected based on the ratio of

carbon associated with ethanol and those associated with the non-alkoxy carbons in the silanol sidechain.

However, [redacted] has a very low solubility (water solubility <0.1 mg/l at 20°C) and may not have fully dissolved and thus not been available for biodegradation in the tests.

The biodegradation observed in the key study is attributable to the biodegradation of the ethanol hydrolysis product. No significant biodegradation is expected for the silanol hydrolysis product. However, as discussed for polydimethylsiloxanes in general, adsorption to sludge can be expected to a high degree.[3]

4 CONCLUSION

The new polymer is not classified as hazardous for human health.

Based on the intended use conditions there is no unforeseeable risk that is not covered by routine hygienic measures to control aerosol exposure.

During service life of cured mixtures no critical risk to human health can be identified.

Regarding the environment neither the hydrolysis product of the monomer nor a similar polymer indicated an acute or chronic environmental concern for the new polymer.

[3] http://www.ecetoc.org/wp-content/uploads/2014/08/JACC-055-Linear-Polydimethylsiloxanes-CAS-No.-63148-62-9-Second-Edition.pdf

5 REFERENCES

BSL Bioservice (2000a). Acute Dermal Irritation/Corrosion with Wacker BS 1701. Testing laboratory: BSL Bioservice Scientific Laboratories GmbH. Report no.: 001695. Owner company: Wacker. Report date: 2000-12-12.

BSL Bioservice. (2001a). Acute Dermal Toxicity (Limit Test) with Wacker BS 1701. Testing laboratory: Bioservice Scientific Laboratories GmbH. Report no.: 001697. Owner company: Wacker. Report date: 2001-01-25.

BSL Bioservice (2001b). Acute Eye Irritation/Corrosion with Wacker BS 1701. Testing laboratory: BSL Bioservice Scientific Laboratories GmbH. Report no.: 001958. Owner company: Wacker. Report date: 2001-01-17.

BSL Bioservice (2001c). Test for Sensitization (Guinea-pig Maximisation Test) with Wacker BS 1701. Testing laboratory: Bioservice Scientific Laboratories GmbH. Report no.: 001696. Owner company: Wacker. Report date: 2001-01-29.

BSL Bioservice (2001d). Repeated Dose Toxicity: 28-day Oral Toxicity Study in Rats with Wacker BS 1701. Testing laboratory: BSL Bioservice Scientific Laboratories GmbH. Report no.: 001699. Owner company: Wacker. Report date: 2001-02-28.

BSL Bioservice. (2001e). In vitro mammalian chromosome aberration test. Testing laboratory: BSL Bioservice Scientific Labs GmbH, Behringstrasse 6, D-82152 Planegg/Munich, Germany. Owner company: Wacker. Study number: 20070723103652467. Report date: 2001-02-27.

Bioservice. (2012). In vitro Mammalian Cell Gene Mutation Assay (Thymidine Kinase Locus/TK+/-) in Mouse Lymphoma L5178Y Cells with [redacted]. Testing laboratory: BSL BIOSERVICE Scientific Laboratories GmbH Behringstraße 6/8 82152 Planegg Germany. Report no.: 115049. Owner company: ReachCentrum SPRL Reconsile Consortium Avenue E. van Nieuwenhuyse 6 1160 Brussels Belgium. Report date: 2012-06-24.

BSL Bioservice. (2015). 90-Day Repeated Dose Oral Toxicity Study in Wistar Rats with [redacted] including a 28-Day Recovery Period. Testing laboratory: BSL Bioservice. Owner company: Reconsile. Study number: 134457. Report date: 2015-09-18.

Bioservice. (2001). Mammalian micronucleus test of murine bone marrow cells. Testing laboratory: Bioservice Scientific Labs GmbH, Behringstrasse 6, D-82152 Planegg, Munich, Germany. Report no.: 1702. Owner company: Wacker. Study number: 001702. Report date: 2001-02-26.

CERI (2001). BS1701 28-day oral toxicity study (full title unknown). Testing laboratory: Chemicals Evaluation and Research Institute, Japan. Report no.: B11-0652. Owner company: Wacker. Study number: 20100531 124828278.

Clarke, N. (2009). SILRES BS 1701: Assessment of Ready Biodegradability; CO2 in sealed vessels. Testing laboratory: Harlan Laboratories Ltd., Shardlow Business Park, Shardlow, Derbyshire. DE72 2GD. Report no.: 2711-0001. Owner company: Wacker.

Dow Corning Corporation (2010). Combined repeated dose toxicity study with the reproductive/developmental toxicity screening test for [redacted] in Sprague-Dawley rats via oral gavage. Testing laboratory: Dow Corning Corporation, Health and environmental Sciences, 2200 W. Salzburg Road, Auburn, MI 48611. Owner company: SEHSC. Study number: 10709-102. Report date: 2010-03-02.

CERI Japan (2001). Report on Mammalian Chromosome Aberration for BS 1701. Testing laboratory: Chemical Evaluation and Research Institute, Japan. Owner company: Wacker. Study number: 20070723124951608. Report date: 2001-08-01.

Harlan (2009a). SILRES® BS 1701: Prenatal Developmental Toxicity Study in the Han Wistar Rat. Harlan Laboratories Ltd. Testing laboratory: Harlan Laboratories Ltd., Fullinsdorf, Switzerland. Report no.: C16992. Owner company: Wacker. Report date: 2009-10-29.

Harlan. (2010a). Effect of SILRES® BS 1701 on Survival and Reproduction of Daphnia magna in a Semi-Static Test over Three Weeks. Testing laboratory: Harlan Laboratories Ltd., Zelgliweg 1, 4452 Itingen, Switzerland. Owner company: Wacker. Study number: Harlan Laboratories Study C17036. Report date: 2010-08-16.

Harlan. (2010b). SILRES® BS 1701: Toxicity to Pseudokirchneriella subcapitata in a 72-Hour Algal Growth Inhibition Test. Testing laboratory: Harlan Laboratories Ltd. Zelgliweg 1 4452 Itingen / Switzerland. Owner company: Wacker Chemie AG, Johannes-Hess-Str. 24 84489 Burghausen / Germany. Study number: Harlan Laboratories Study C17025. Report date: 2010-08-17.

Hertl, J. (2001). Ready biodegradability of Wacker BS 1701 in a manometric respirometry test. Testing laboratory: Institut fur Biologische Analytik und Consulting IBACON GmnB, Arheilger Weg 17, 64380 Rossdorf, Germany. Report no.: 9545160. Owner company: Wacker. Report date: 2001-01-22.

Hoechst (1986a). [redacted] - Akute Aerosolinhalation an männlichen und weiblichen SPF-Wistar Ratten - 4 stunden LC50. Testing laboratory: Hoechst - Pharma Forschung Toxikologie. Report no.: 15422/9/02. Report date: 1986-10-01.

Hoechst (1986b). [redacted]: Subakute inhalative Toxizität - 20 Expositionen in 28 Tagen an SPF-Wistar-Ratten. Testing laboratory: Hoechst Pharma Forschung Toxikologie und Pathologie. Report no.: 86.0852. Owner company: Wacker-Chemie GmbH. Report date: 1986-10-01.

IBACON (2001a). Additional study on Acute Toxicity of Wacker BS 1701 to Rainbow Trout (Oncorhynchus mykiss) in a 96-hour Static Test. Testing laboratory: IBACON GmbH, Rossdorf, Germany. Owner company: Wacker. Study number: 9543230. Report date: 2001-03-14.

IBACON (2001b). Acute Toxicity of Wacker BS 1701 to Rainbow Trout (Oncorhynchus mykiss) in a 96-hour Static Test. Testing laboratory: IBACON GmbH, Rossdorf, Germany. Owner company: Wacker. Study number: 9543230. Report date: 2001-03-09.

IBACON (2001c). Acute Toxicity of Wacker BS 1701 to Daphnia magna in a 48-hour Immobilization Test. Testing laboratory: IBACON GmbH, Rossdorf, Germany. Owner company: Wacker. Study number: 9541220. Report date: 2001-03-08.

IBACON (2001d). Additional study on Acute Toxicity of Wacker BS 1701 to Daphnia magna in a 48-hour Immobilization Test. Testing laboratory: IBACON GmbH, Rossdorf, Germany. Owner company: Wacker-Chemie GmbH. Study number: 9541220. Report date: 2001-03-19.

OECD. (2004). SIDS Initial Assessment Report for SIAM 19, Berlin, Germany, 19-22 October 2004, Ethanol, CAS 64-17-5.

RCC (1998). Wacker BS 1701: Acute Oral Toxicity Study in Rats. Testing laboratory: Research and Consulting Company Ltd. Report no.: 688983. Owner company: Wacker. Report date: 1998-06-29.

RCC Cytotest Cell Research GmbH (1998). 20070723104404022. pdf. Testing laboratory: RCC Cytotest Cell Research GmbH, In den Leppsteinswiesen 19, D-64380 Rossdorf, Germany. Report no.: 605900. Owner company: Wacker. Report date: 1998-05-12.

Springborn Smithers. (2008a). [redacted] - Acute Toxicity to Rainbow Trout (Oncorhynchus mykiss) Under Flow-Through Conditions, Following OECD Guideline Number 203. Testing laboratory: Springborn Smithers Laboratories, Wareham, Massachusetts, USA. Owner company: SEHSC. Study number: Springborn Smithers - 12023.6168. Report date: 2008-07-24.

Springborn Smithers. (2008b). [redacted] - Acute Toxicity to Water Fleas, Daphnia magna, Under Flow-Through Conditions, Following OECD Guideline Number 202. Testing laboratory: Springborn Smithers Laboratories, Wareham, Massachusetts, USA. Owner company: SEHSC. Study number: Springborn Smithers - 12023.6167. Report date: 2008-08-19.

Springborn Smithers (2008c). [redacted] – 72-Hour Acute Toxicity Test with Freshwater Green Alga, Pseudokirchneriella subcapitata. Testing laboratory: Springborn Smithers Laboratories 790 Main Street Wareham, Massachusetts 02571-1037, USA. Owner company: SEHSC. Study number: Springborn Smithers Study No. 12023.6166. Report date: 2008-09-17.

6 ANNEX I – MPBPWIN V1.43 CALCULATIONS

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Experimental Database Structure Match:  no data

[redacted]
CHEM   :
[redacted]
MOL WT : 276.50
----------------------- SUMMARY MPBPWIN v1.43 --------------------


Boiling Point:  268.81 deg C (Adapted Stein and Brown Method)

Melting Point:   36.35 deg C (Adapted Joback Method)
Melting Point:   43.29 deg C (Gold and Ogle Method)
Mean Melt Pt :   39.82 deg C (Joback; Gold,Ogle Methods)
  Selected MP:   39.82 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
  (Using BP: 268.81 deg C (estimated))
  (Using MP: 39.82 deg C (estimated))
    VP:  0.00708 mm Hg (Antoine Method)
       :  0.944 Pa  (Antoine Method)
    VP:  0.00739 mm Hg (Modified Grain Method)
       :  0.985 Pa  (Modified Grain Method)
    VP:  0.013 mm Hg (Mackay Method)
       :  1.74 Pa  (Mackay Method)
  Selected VP:  0.00739 mm Hg (Modified Grain Method)
             :  0.985 Pa (Modified Grain Method)
  Subcooled liquid VP:  0.0101 mm Hg (25 deg C, Mod-Grain method)
                     :  1.34 Pa  (25 deg C, Mod-Grain method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  7  |  -CH3              |   21.98  |  153.86
 Group |  5  |  -CH2-             |   24.22  |  121.10
 Group |  1  |  >CH-              |   11.86  |   11.86
 Group |  1  |  >C<               |    4.50  |    4.50
 Group |  3  |  -O- (nonring)     |   25.16  |   75.48
 Group |  1  |  Si (non-ring)     | regress  |    3.92
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  568.90
RESULT- corr |  BOILING POINT in deg Kelvin  |  541.97
             |  BOILING POINT in deg C       |  268.81
-------------------------------------------------------

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  7  |  -CH3              |   -5.10  |  -35.70
 Group |  5  |  -CH2-             |   11.27  |   56.35
 Group |  1  |  >CH-              |   12.64  |   12.64
 Group |  1  |  >C<               |   46.43  |   46.43
 Group |  3  |  -O- (nonring)     |   22.23  |   66.69
 Group |  1  |  Si (non-ring)     | regress  |   40.60
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  309.51
             |  MELTING POINT in deg C       |   36.35
-------------------------------------------------------


Experimental Database Structure Match:  no data

[redacted]
CHEM   :
[redacted]
MOL WT : 478.87
----------------------- SUMMARY MPBPWIN v1.43 --------------------


Boiling Point:  399.39 deg C (Adapted Stein and Brown Method)

Melting Point:  170.86 deg C (Adapted Joback Method)
Melting Point:  119.54 deg C (Gold and Ogle Method)
```

```
Mean Melt Pt :  145.20 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  136.65 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
  (Using BP: 399.39 deg C (estimated))
  (Using MP: 136.65 deg C (estimated))
    VP:  1.39E-007 mm Hg (Antoine Method)
       :  1.85E-005 Pa  (Antoine Method)
    VP:  6.47E-007 mm Hg (Modified Grain Method)
       :  8.62E-005 Pa  (Modified Grain Method)
    VP:  1.39E-006 mm Hg (Mackay Method)
       :  0.000185 Pa  (Mackay Method)
  Selected VP:  6.47E-007 mm Hg (Modified Grain Method)
              :  8.62E-005 Pa (Modified Grain Method)
  Subcooled liquid VP:  8.6E-006 mm Hg (25 deg C, Mod-Grain method)
                     :  0.00115 Pa  (25 deg C, Mod-Grain method)
```

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	12	-CH3	21.98	263.76
Group	8	-CH2-	24.22	193.76
Group	2	>CH-	11.86	23.72
Group	2	>C<	4.50	9.00
Group	5	-O- (nonring)	25.16	125.80
Group	2	Si (non-ring)	regress	-0.50
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		813.72
RESULT- corr		BOILING POINT in deg Kelvin		672.55
		BOILING POINT in deg C		399.39

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	12	-CH3	-5.10	-61.20
Group	8	-CH2-	11.27	90.16
Group	2	>CH-	12.64	25.28
Group	2	>C<	46.43	92.86
Group	5	-O- (nonring)	22.23	111.15
Group	2	Si (non-ring)	regress	63.27
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		444.02
		MELTING POINT in deg C		170.86

ANNEX II – ECOSAR Calculations

ECOSAR Version 1.11 Results Page

[redacted]
CHEM :
CAS Num:
ChemID1:
[redacted]
MOL WT : 192.33
Log Kow: 0.890 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: (User Entered for Wat Sol estimate)
Melt Pt: (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 8314 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: (PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 0.890 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 8314 (mg/L, EPISuite WSKowwin v1.43 Estimate)

ECOSAR v1.11 Class-specific Estimations

****

Not Related to an Existing ECOSAR Class Definition
Estimates provided below use the Neutral Organics QSAR equations which represent baseline toxicity potential (minimum toxicity) assuming a simple non-polar narcosis model. Without empirical data on structurally similar chemicals, it is uncertain if this substance will present significantly higher toxicity above baseline estimates.

****

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	Fish	96-hr	LC50	1568.714
Neutral Organics	Daphnid	48-hr	LC50	803.957
Neutral Organics	Green Algae	96-hr	EC50	392.008
Neutral Organics	Fish		ChV	135.875
Neutral Organics	Daphnid		ChV	58.946
Neutral Organics	Green Algae		ChV	81.709
Neutral Organics	Fish (SW)	96-hr	LC50	1961.814
Neutral Organics	Mysid	96-hr	LC50	3092.571
Neutral Organics	Fish (SW)		ChV	108.115
Neutral Organics	Mysid (SW)		ChV	371.430
Neutral Organics	Earthworm	14-day	LC50	435.873

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

ECOSAR Version 1.11 Results Page

[redacted]
CHEM   :
CAS Num:
ChemID1:
[redacted]
MOL WT : 715.28
Log Kow: 9.842   (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: (User Entered for Wat Sol estimate)
Melt Pt: (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 3.078E-007 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: (PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 9.842   (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 3.078E-007 (mg/L, EPISuite WSKowwin v1.43 Estimate)

ECOSAR v1.11 Class-specific Estimations

| Not Related to an Existing ECOSAR Class Definition |
| Estimates provided below use the Neutral Organics QSAR equations which represent baseline toxicity potential (minimum toxicity) assuming a simple non-polar narcosis model. Without empirical data on structurally similar chemicals, it is uncertain if this substance will present significantly higher toxicity above baseline estimates. |

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	Fish	96-hr	LC50	5.33e-005 *
Neutral Organics	Daphnid	48-hr	LC50	6.24e-005 *
Neutral Organics	Green Algae	96-hr	EC50	0.000927 *
Neutral Organics	Fish		ChV	1.22e-005 *
Neutral Organics	Daphnid		ChV	4.56e-005 *
Neutral Organics	Green Algae		ChV	0.00122 *
Neutral Organics	Fish (SW)	96-hr	LC50	7.03e-005 *
Neutral Organics	Mysid	96-hr	LC50	2.58e-007
Neutral Organics	Fish (SW)		ChV	0.000916 *
Neutral Organics	Mysid (SW)		ChV	2.18e-009
Neutral Organics	Earthworm	14-day	LC50	191.198 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)

Maximum LogKow: 8.0 (ChV)